PATENT APPLICATION

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re application of

Express Mail No. EF279046015US

Richard James GILBERT et al.

Filed: November 16, 2001

For: METHOD FOR GENERATING A DATABASE OF MOLECULAR FRAGMENTS

PRELIMINARY AMENDMENT

Commissioner for Patents
Washington, D.C. 20231

Sir:

Prior to examination and **prior to calculation of the filing fee**, please amend the above-identified application as follows:

IN THE CLAIMS:

Please enter the following amended claims:

4. (Amended) A method according to claim 3, wherein the maximum common structure is the maximum molecular structure of atoms bonded as a single connected entity.

5. (Amended) A method according to claim 1, further comprising a step of comparing the molecular fragment data determined in step (b) with the molecular structure data already within the data set and subsequently storing the determined molecular fragment data only if molecular structure data defining an identical molecular structure is not already present within the data set.

7. (Amended) A method according to claim 1, wherein the determined molecular fragment data comprises data identifying the first or second molecular structure data which has been involved

in any previous comparison steps which have resulted in the determination of that particular molecular fragment data.

9. (Amended) A method according to claim 7, further comprising a step of comparing the molecular fragment data determined in step (b) with the molecular structure data already within the data set and subsequently storing the determined molecular fragment data only if molecular structure data defining an identical molecular structure is not already present within the data set, wherein, if the determined molecular fragment as defined by the molecular fragment data, is found to be identical to a molecular structure as defined by corresponding molecular structure data already present within the data set, the identifying data is added to the molecular structure data defining the molecular structure that is already present within the data set.

10. (Amended) A method according to claim 1 wherein step (b) is performed using a method according to graph theory.

12. (Amended) A method according to claim 1 further comprising ranking the molecular structure data in the data set according to the frequency with which molecular structures identical to each particular molecular structure have been determined, and discarding the molecular structure data defining molecular structures which occur less frequently than a predetermined frequency threshold.

13. (Amended) A method according to claim 12, wherein only a number of the molecular fragment data are retained within the database.

14. (Amended) A method according to claim 1, further comprising:

e) comparing the molecular fragment data in the database with molecular structure data defining each of the predetermined molecular structures; and

f) determining the frequency of occurrence of each molecular fragment within each predetermined molecular structure.

20. (Amended) A method according to claim 18, wherein the step of determining the relationship is performed using a numerical model.

21. (Amended) A computer implemented method of generating predicted biological target characteristic data for a target molecule, the method comprising:-

obtaining target molecular structure data defining the molecular structure of the target molecule;

obtaining the relationship between the presence of a number of molecular fragments in a number of molecular structures and a biological target characteristic of the molecular structures, the method comprising:-

obtaining a modelling data set comprising data defining the molecular structures of a number of known molecules and corresponding known biological target characteristic data defining a common biological target characteristic for each molecule;

obtaining a database of molecular fragments data generated using a method according to any of the preceding claims;

obtaining data describing the presence of the molecular structures defined by the molecular fragment data, within the known molecules of the modelling data set; and,

determining a relationship between the data describing the presence of a number of the molecular fragments within the known molecules of the modelling data set and the common biological target characteristic data;

processing the target molecular structure data to generate target fragment data describing the presence within the target molecule, of the molecular structures defined by the molecular fragment data used in the obtained relationship; and,

using the obtained relationship and the target fragment data to generate biological target characteristic data for the target molecule.

22. (Amended) A method according to claim 21, wherein the molecular structure of the target molecule is different from the molecular structures of the known molecules or the molecules used in the generation of the molecular fragment data.

26. (Amended) A method according to claim 23, wherein a number of the known molecules have identical structures to a number of the molecular structures used in the generation of the molecular fragment data.

27. (Amended) A method according to claim 23, wherein the step of determining the relationship is performed using a numerical model.

28. (Amended) A computer implemented method of generating biological target characteristic data for a target molecule, the method comprising:-

obtaining target molecular structure data defining the molecular structure of the target molecule;

obtaining the relationship generated in the method of determining a relationship between the presence of a number of molecular fragments in a number of molecular structures and a biological target characteristic, the method comprising:-

obtaining a modelling data set comprising data defining the molecular structures of a number of known molecules and corresponding known biological target characteristic data defining a common biological target characteristic for each molecule;

obtaining a database of molecular fragment data:

obtaining data describing the frequency of occurrence of a number of the molecular structures defined by the molecular fragment data, within the known molecules

of the modelling data set wherein the data contains at least one non-integer frequency of occurrence; and

determining a relationship between the data describing the frequency of occurrence of the molecular fragments within the known molecules of the modelling data set and the common biological target characteristic data.;

processing the target molecular structure data to generate target fragment data describing the presence within the target molecule, of the molecular structures defined by the molecular fragment data used in the obtained relationship wherein the presence includes at least one non-integer frequency of occurrence; and,

using the obtained relationship and the target fragment data to generate biological target characteristic data for the target molecule.

29. (Amended) A method according to claim 28, wherein the molecular structure of the target molecule is different from the molecular structures of the known molecules or the molecules used in the generation of the molecular fragment data.

30. (Amended) A computer program comprising program code means adapted to perform the method according to claim 28, when the computer program is run on a computer.

REMARKS

The foregoing amendments have been made to ensure correct dependencies in the claims, and only correct obvious typographical errors. None of these changes has been made for reasons of patentability under any provision of Title 35, U.S.C. Early, favorable consideration on the merits is respectfully requested.

Respectfully submitted,

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APPENDIX

VERSION WITH MARKINGS TO SHOW CHANGES MADE

IN THE CLAIMS:

The claims are amended as follows:

4. (Amended) A method according to [claim 2 or] claim 3, wherein the maximum common structure is the maximum molecular structure of atoms bonded as a single connected entity.

5. (Amended) A method according to [any of the preceding claims] claim 1, further comprising a step of comparing the molecular fragment data determined in step (b) with the molecular structure data already within the data set and subsequently storing the determined molecular fragment data only if molecular structure data defining an identical molecular structure is not already present within the data set.

7. (Amended) A method according to [any of the preceding claims] claim 1, wherein the determined molecular fragment data comprises data identifying the first or second molecular structure data which has been involved in any previous comparison steps which have resulted in the determination of that particular molecular fragment data.

9. (Amended) A method according to [claims 7 or claim 8] claim 7, [and when dependent upon claim 5,] further comprising a step of comparing the molecular fragment data determined in step

(b) with the molecular structure data already within the data set and subsequently storing the determined molecular fragment data only if molecular structure data defining an identical molecular structure is not already present within the data set, wherein, if the determined molecular fragment as defined by the molecular fragment data, is found to be identical to a molecular structure as defined by corresponding molecular structure data already present within the data set, the identifying data is added to the molecular structure data defining the molecular structure that is already present within the data set.

10. (Amended) A method according to [any of the preceding claims] claim 1 wherein step (b) is performed using a method according to graph theory.

12. (Amended) A method according to [any of the preceding claims] claim 1 further comprising ranking the molecular structure data in the data set according to the frequency with which molecular structures identical to each particular molecular structure have been determined, and discarding the molecular structure data defining molecular structures which occur less frequently than a predetermined frequency threshold.

13. (Amended) A method according to claim [13] 12, wherein only a number of the molecular fragment data are retained within the database.

14. (Amended) A method according to [any of the preceding claims] claim 1, further comprising:

[f)] e) comparing the molecular fragment data in the database with molecular structure data defining each of the predetermined molecular structures; and

[g)] f) determining the frequency of occurrence of each molecular fragment within each predetermined molecular structure.

20. (Amended) A method according to claim 18 [or claim 19], wherein the step of determining the relationship is performed using a numerical model.

21. (Amended) A computer implemented method of generating predicted biological target characteristic data for a target molecule, the method comprising:-

obtaining target molecular structure data defining the molecular structure of the target molecule;

obtaining the relationship [generated in the method according to any of claims 18 to 20] between the presence of a number of molecular fragments in a number of molecular structures and a biological target characteristic of the molecular structures, the method comprising:-

obtaining a modelling data set comprising data defining the molecular structures of a number of known molecules and corresponding known biological target characteristic data defining a common biological target characteristic for each molecule;

obtaining a database of molecular fragments data generated using a method according to any of the preceding claims;

obtaining data describing the presence of the molecular structures defined by the molecular fragment data, within the known molecules of the modelling data set; and,

determining a relationship between the data describing the presence of a number of the molecular fragments within the known molecules of the modelling data set and the common biological target characteristic data;

processing the target molecular structure data to generate target fragment data describing the presence within the target molecule, of the molecular structures defined by the molecular fragment data used in the obtained relationship; and,

using the obtained relationship and the target fragment data to generate biological target characteristic data for the target molecule.

22. (Amended) A method according to claim 21, wherein the molecular structure of the target molecule is different [to] from the molecular structures of the known molecules or the molecules used in the generation of the molecular fragment data.

26. (Amended) A method according to [any of claims 23 to 25] claim 23, wherein a number of the known molecules have identical structures to a number of the molecular structures used in the generation of the molecular fragment data.

27. (Amended) A method according to [any of claims 23 to 26] claim 23, wherein the step of determining the relationship is performed using a numerical model.

28. (Amended) A computer implemented method of generating biological target characteristic data for a target molecule, the method comprising:-

obtaining target molecular structure data defining the molecular structure of the target molecule;

obtaining the relationship generated in the method [according to any of claims 23 to 27] of determining a relationship between the presence of a number of molecular fragments in a number of molecular structures and a biological target characteristic, the method comprising:-

obtaining a modelling data set comprising data defining the molecular structures of a number of known molecules and corresponding known biological target characteristic data defining a common biological target characteristic for each molecule;

obtaining a database of molecular fragment data:

obtaining data describing the frequency of occurrence of a number of the molecular structures defined by the molecular fragment data, within the known molecules of the modelling data set wherein the data contains at least one non-integer frequency of occurrence; and

determining a relationship between the data describing the frequency of occurrence of the molecular fragments within the known molecules of the modelling data set and the common biological target characteristic data.;

processing the target molecular structure data to generate target fragment data describing the presence within the target molecule, of the molecular structures defined by the molecular fragment data used in the obtained relationship wherein the presence includes at least one non-integer frequency of occurrence; and,

using the obtained relationship and the target fragment data to generate biological target characteristic data for the target molecule.

29. (Amended) A method according to claim 28, wherein the molecular structure of the target molecule is different [to] from the molecular structures of the known molecules or the molecules used in the generation of the molecular fragment data.

30. (Amended) A computer program comprising program code means adapted to perform the method according to [any of preceding claims] claim 28, when the computer program is run on a computer.